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Comparing Natural Product (NP) and non-NP datasets at an atomic scale

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Understanding the basic chemical composition of secondary natural products (NP) will help to design NP like agents more efficiently. This should lead to an elaborated comprehension of the biosynthetic origin of natural products and to an efficient way to simulate and to imitate these structures in research and development, especially since it is known that natural and natural like products differ from non natural synthetic compounds to some extent [1].

Initial research regarding the comparative analysis of natural products, synthetic compounds, and drugs has already been done in 1999 [2], and more recently this year [3]. Additionally, a statistical analysis of natural macrocycles has been performed lately [4], ring systems were examined with respect of their structural similarities [5] by charting natural products in general [6]. A different analysis concerning natural products versus molecules from combinatorial synthesis with respect to drug design was done in 2003 [7].

In order to capture the evolutionary advantage of NPs, it is of high relevance to develop methods for their differentiation from chemical molecules in general, separating NPs and NP-like compounds out of the set of all chemical structures. Despite of the previously done comparisons between natural product compounds and synthetic ones, here we present a general comparison of all elements and atom types for an advanced classification of compounds from different resources. These results will be the basis for all kind of further, more detailed analyses with regard to drug alikeness and development. Cheminformatic analysis of the frequency of selected structural elements occurring in natural products in comparison to compounds of synthetic origin should gain more insight in essential differences between both classes of compounds. For this purpose, a JAVA application was developed to examine eight datasets of various vendors, with three among them containing natural products only. These data were analysed to understand - on an atomic scale - the differences between compounds synthesised by nature and compounds synthesised by man.

References

1. Ortholand J-Y, Ganesan A: *Curr Op Chem Bio* 2004:271.
2. Henkel T, Brunne RM, Müller H, Reichel F: *Angew. Chem.* 1999:688.
3. Grabowski K, Schneider G: *Curr Chem Biol* 2007:115.
4. Wessjohann LA, Ruijter E, Garcia-Rivera D, Brandt W: *Mol. Divers* 2005:171.
5. Lee M-L, Schneider G: *J Comb Chem* 2001:284.
6. Koch MA, Schuffenhauer A, Scheck M, Wetzel S, Casaulta M, Odermatt A, Ertl P, Waldmann H: *PNAS* 2005:17272.
7. Feher M, Schmidt JM: 2003:218.